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New numerical integrator for the Stäckel system conserving the same number of constants of motion as the degree of freedom

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Abstract

A new numerical integrator for a wide class of separable Hamiltonian systems called the Stäckel system is presented. This integrator is designed so as to conserve the same number of constants of motion as the degree of freedom of the Stäckel system. Separation of variables of the Stäckel system is most fundamental for the integrator. A combination of canonical transformations and an energy-preserving method with a variable step-size plays a key role to design such an integrator. Some typical and important examples of the Stäckel system are then discretized explicitly. They are the three-dimensional Kepler motion, the Holt system and the integrable Henon–Heiles system in celestial mechanics.

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1. Introduction

Many numerical integrators for dynamical systems have been studied in order to well approximate the continuous-time orbits. To investigate the long-time behaviour, several structured integrators are quite useful.

The symplectic integrators (cf [8, 26]) are numerical integration schemes for Hamiltonian systems, which conserve the symplectic form in the phase space, so that the resulting discrete-time evolution is regarded as a canonical transformation. Though the symplectic integrators do not conserve Hamiltonian and other additional constants of motion, in general, they are widely used in numerical simulation for various Hamiltonian systems. This is because the symplectic integrators give a good approximation of orbits of the Hamiltonian system in the sense in which they conserve a modified (or approximate) Hamiltonian.

The energy-preserving method was presented by Greenspan [4, 5]. This method keeps the value of discrete energy constant for any step-size. In particular, explicit energy-preserving schemes were developed for Hamiltonian systems with at most quartic potential in [13].

Recently, various integrators based on the discrete variational principle have been designed. These integrators are classified into symplectic-momentum integrators and energy–momentum integrators. Symplectic-momentum integrators [31, 33] for Lagrangian systems keep a symplectic form and conserve a discrete momentum derived through a discrete Noether theorem. An energy–momentum integrator for Lagrangian systems is designed in [21]. Gonzalez presented energy–momentum integrators for Hamiltonian systems in [7]. Energy–momentum integrators keep the values of energy and discrete momenta. Regarding a time variable as a coordinate, a symplectic-energy–momentum integrator was recently presented in [14]. This integrator conserves the values of a discrete energy and a discrete momentum, and keeps the symplectic form. The symplectic-momentum integrators and the energy–momentum integrators preserve the values of modified constants of motion different from the original ones. These modified constants are derived from a discrete Noether theorem.

A Hamiltonian system with n degrees of freedom is said to be completely integrable if it has n constants of motion in involution, which are functionally independent. This is the context of Liouville–Arnold theorem [24]. However, some of such constants are not always derived from a discrete Noether theorem. Hence, for the above integrators, it seems difficult to simulate a long-term behaviour of such a completely integrable Hamiltonian system with a sufficient accuracy. Actually, these integrators do not always give accurate behaviours of the original integrable systems. For example [34, 35], the Runge–Lenz vector of the Kepler motion is not conserved by a symplectic integrator. Therefore, the pericentre of the elliptic orbit moves.

A set of n functionally independent constants of motion, which an n-dimensional completely integrable Hamiltonian system preserves, fixes a single orbit on a phase space. It is hopeful that an integrator is designed to conserve exactly n constants which an n-dimensional completely integrable Hamiltonian system has.

An exact conservative integrator for the n-body problem including the Kepler problem which conserves the Hamiltonian and the angular momentum is presented in [16]. Shadwick, Bowman and Morrison [27] presented an integration scheme for the Kepler motion conserving the Hamiltonian and the Runge–Lenz vector. However, the resulting integrator seems to be numerically unstable for a large step-size. It has not been known for a long time how to design an energy-preserving method which is stable and conserves all of the additional constants of motion of a wide class of completely integrable Hamiltonian systems.

Recently, the authors [22] presented the two-dimensional discrete Kepler motion by taking the Levi-Civita regularization theory [1, 20, 28] together with an energy-preserving method for the two-dimensional harmonic oscillator with a variable step-size. Then the original Hamiltonian, the angular momentum and the Runge–Lenz vector are conserved exactly under the time evolution of the discrete Kepler motion. Since all the constants of motion take constant values, the orbit of the discrete Kepler motion correctly traces an ellipse, a parabola or a hyperbola according to the initial value. In the second paper [23], the three-dimensional Kepler motion is discretized by the same numerical integration scheme. The Kustaanheimo–Stiefel (KS) regularization theory [17, 28] plays a central role in [23]. It is to be noted that the two- and three-dimensional discrete Kepler motions found in [22, 23] are stable explicit schemes and a variable step-size is easily introduced.

The idea of applying the KS regularization technique to numerical calculation is not new. Such a technique was already proposed in Bettis [2] in 1970. An exact integration scheme for the Kepler motion based on an exact discretization of the harmonic oscillator and the KS regularization transformation was given. The resulting scheme is shown to be numerically stable. However, any explicit recurrence relation and any conservation of the constants of motion were not discussed. The KS transformation and its application was also discussed in [1, 32]. With the help of the transformation, a time-reversible integrator which conserves all constants of motions of the Kepler motion has been derived by Leimkuhler [19] in 1999. A transformation of the discrete time in [19], which is a discrete analogue of the Kepler change of the time, is different from that in [22, 23]. Though this transformation guarantees the time-reversibility, it makes the integrator implicit.

The new numerical integration scheme in [22, 23] is based on an energy-preserving method and canonical transformations into separable Hamiltonian systems called the Levi-Civita and KS transformation. The next challenging problem is to make clear the essence and a coverage of the new scheme. The purpose of this paper is twofold. This paper shows that

(I) the new numerical integrator is applicable to a wide class of Hamiltonian systems called the Stäckel system;

(II) separation of variables is essential to find such a numerical integrator that conserves the same number of constants of motion as the degree of freedom of the Stäckel system.

The Stäckel system is known as the most general class of separable Hamiltonian systems which includes the Liouville system [24]. The Stäckel system has the same number of constants of motion as the degree of freedom. The main idea of this paper is to apply the energy-preserving method with a variable step-size to Hamiltonian systems whose variables can be separated by using certain canonical transformations. To this end, an extended phase space [18, 29] is introduced, where a time variable and a minus Hamiltonian give a conjugate pair of canonical variables. Then, a numerical integrator is designed which conserves the same number of constants of motion as the degree of freedom of the Stäckel system. It is shown that certain canonical transformations which separate canonical variables are quite useful as well as the regularization transformations. We then illustrate our integrator by applying it to the three-dimensional Kepler motion, the Holt system and an integrable Henon–Heiles system. The Kepler motion and the Henon–Heiles system are important examples of the Stäckel system which appear in celestial mechanics. An accurate numerical integrator is especially needed to simulate long-time behaviours of solutions.

This paper is organized as follows. In section 2, a review of the basic properties of the Stäckel system and its duality and canonical transformations is given. Typical and important examples of the Stäckel system are the three-dimensional Kepler motion, the Holt system and the integrable Henon–Heiles system. In section 3, it is shown that an energy-preserving scheme for a Hamiltonian expressed by the sum of one-dimensional Hamiltonian systems induces a numerical integrator which conserves the same number of constants of motion as the degree of freedom of a given Stäckel system. An algorithm of the numerical integrator is then described. In section 4, a three-dimensional discrete Kepler motion, a discrete Holt system and a discrete integrable Henon–Heiles system are presented. Each of them keeps at least the same number of constants of motion as its degree of freedom. A difference between the discrete Kepler motion and the integrator in [19] is discussed. Numerical examples are also given for the three-dimensional discrete Kepler motion, the discrete Holt system and the discrete Henon–Heiles system. The orbits remarkably trace the orbits of the continuous-time orbits for rather large discrete step-size.

2. Stäckel system and related completely integrable systems

2.1. Stäckel system

Separation of variables is one of the fundamental methods for integrating equations of motions. It enables us to reduce integration of a system with several degrees of freedom to integration of a sequence of one-dimensional problems. The Stäckel system is an important class of separable Hamiltonian systems having more than two degrees of freedom. Recently, Grigoryev and Tsiganov [6] presented an implementation of the algorithm for finding the separation variables for given integrable systems including Stäckel system. In this paper, we utilize separation of variables to design a new numerical integration algorithm. There is a basic theorem (cf [24], p 101) proposed by Stäckel in 1891.

Theorem 1 (Stäckel)**.** *Let $H(p_1, \ldots, p_N, q_1, \ldots, q_N)$ be a Hamiltonian expressed as*

$$H(p_1, \ldots, p_N, q_1, \ldots, q_N) = \sum_{j=1}^{N} g_j(q_1, \ldots, q_N)\big(p_j^2 + U_j(q_j)\big), \tag{1}$$

where $U_j(q_j)$, $j = 1, \ldots, N$, are the potential functions. A system with the Hamiltonian (1) admits a separation of variables of the corresponding Hamilton–Jacobi equation if and only if there exists a nonsingular $N \times N$ matrix $\mathbf{S} = (s_{i,j})$ whose elements $s_{i,j}$ depend only on q_j such that

$$\sum_{j=1}^{N} s_{i,j}(q_j) g_j(q_1, \ldots, q_N) = \delta_{i,1}. \tag{2}$$

The Hamiltonian system satisfying the property in theorem 1 is called the Stäckel system. The Stäckel system covers a wider class of completely integrable dynamical systems than the Liouville system. The matrix $\mathbf{S}$ is sometimes called the Stäckel matrix. It is to be noted that the first column of the inverse $\mathbf{S}^{-1} = (c_{i,j})$ is expressed as

$$c_{i,1} = g_i(q_1, \ldots, q_N), \qquad i = 1, \ldots, N. \tag{3}$$

If $g_i = g_j$, $i \neq j$, then the Stäckel system is reduced to the Liouville system. Let us define the quantities $I_k = I_k(p_1, \ldots, p_N, q_1, \ldots, q_N)$, $k = 1, \ldots, N$, by

$$\begin{pmatrix} I_1 \\ \vdots \\ I_N \end{pmatrix} = (\mathbf{S}^{-1})^{\top} \begin{pmatrix} p_1^2 + U_1(q_1) \\ \vdots \\ p_N^2 + U_N(q_N) \end{pmatrix}. \tag{4}$$

Proposition 1 (cf [24])**.** *The Stäckel system with the Hamiltonian (1) has the same number of constants of motion as the degree of freedom. The quantities I_k are constants of motion of the Hamiltonian system in involution. Especially, I_1 is just the Hamiltonian $I_1 = H$.*

Thus, the Stäckel systems are completely integrable Hamiltonian systems in the sense of Liouville–Arnold.

2.2. Canonical transformations between Stäckel systems

Let $H = H(p_1, \ldots, p_N, q_1, \ldots, q_N)$ be a Hamiltonian on the $2N$-dimensional phase space $\mathcal{M}$ with the canonical coordinates $\{p_j, q_j\}_{j=1,\ldots,N}$. We extend $\mathcal{M}$ by adding to it the new coordinate $q_{N+1} = t$ and the corresponding momentum $p_{N+1} = -H$. The resulting $(2N+2)$-dimensional space $\mathcal{M}_{\mathcal{E}}$ is the so-called extended phase space of the Hamiltonian system [18, 29]. The energy E is an arbitrary fixed value of the variable H in (1).

To describe time evolution on the extended phase space $\mathcal{M}_{\mathcal{E}}$, we introduce the extended Hamiltonian

$$\mathcal{H}(p_1,\ldots,p_{N+1},q_1,\ldots,q_{N+1}) = H(p_1,\ldots,p_N,q_1,\ldots,q_N) - E. \tag{5}$$

The Hamiltonian system for the variables p_j, q_j, $j = 1,\ldots,N$,

$$\begin{aligned}\frac{\mathrm{d}p_j}{\mathrm{d}t} &= -\frac{\partial\mathcal{H}(p_1,\ldots,p_{N+1},q_1,\ldots,q_{N+1})}{\partial q_j},\\ \frac{\mathrm{d}q_j}{\mathrm{d}t} &= \frac{\partial\mathcal{H}(p_1,\ldots,p_{N+1},q_1,\ldots,q_{N+1})}{\partial p_j},\end{aligned} \tag{6}$$

coincides with the Hamiltonian system given by the original Hamiltonian H. The time variable $q_{N+1} = t$ is a cyclic coordinate and the conjugated momentum $p_{N+1} = -E$ is a constant of motion. Because of $p_{N+1} = -E$,

$$\mathcal{H}(p_1,\ldots,p_{N+1},q_1,\ldots,q_{N+1}) \equiv 0. \tag{7}$$

Namely, $\mathcal{H}$ is identically equal to zero for any t. In this paper, we call (7) a *zero Hamiltonian condition*.

Let us introduce a general extended canonical transformation

$$\begin{aligned}&\{p_1,\ldots,p_N,p_{N+1},q_1,\ldots,q_N,q_{N+1}\} \mapsto \{p_1,\ldots,p_N,\widetilde{p}_{N+1},q_1,\ldots,q_N,\widetilde{q}_{N+1}\},\\ &p_{N+1} = -E, \qquad \widetilde{p}_{N+1} = -\widetilde{E}, \qquad q_{N+1} = t, \qquad \widetilde{q}_{N+1} = \widetilde{t}\end{aligned} \tag{8}$$

on the extended phase space $\mathcal{M}_{\mathcal{E}}$ such that

$$\begin{aligned}&E \mapsto \widetilde{E}, \qquad \widetilde{E} = \frac{E}{v(p_1,\ldots,p_N,q_1,\ldots q_N)},\\ &t \mapsto \widetilde{t}, \qquad \mathrm{d}\widetilde{t} = v(p_1,\ldots,p_N,q_1,\ldots q_N)\,\mathrm{d}t,\end{aligned} \tag{9}$$

where $v(p_1,\ldots,p_N,q_1,\ldots,q_N)$ is a nonzero function on the phase space $\mathcal{M}$. The transformation (8) changes the original Hamiltonian system (6) on $\mathcal{M}$ to

$$\begin{aligned}\frac{\mathrm{d}p_j}{\mathrm{d}\widetilde{t}} &= -\frac{1}{v(p_1,\ldots,p_N,q_1,\ldots,q_N)}\frac{\partial\mathcal{H}}{\partial q_j},\\ \frac{\mathrm{d}q_j}{\mathrm{d}\widetilde{t}} &= \frac{1}{v(p_1,\ldots,p_N,q_1,\ldots,q_N)}\frac{\partial\mathcal{H}}{\partial p_j},\end{aligned} \tag{10}$$

but conserves the form of the Hamiltonian system on the extended phase space $\mathcal{M}_{\mathcal{E}}$ because of condition (7)

$$\begin{aligned}\frac{\mathrm{d}p_j}{\mathrm{d}\widetilde{t}} &= -\frac{\partial\widetilde{\mathcal{H}}(p_1,\ldots,p_N,\widetilde{p}_{N+1},q_1,\ldots,q_N,\widetilde{q}_{N+1})}{\partial q_j},\\ \frac{\mathrm{d}q_j}{\mathrm{d}\widetilde{t}} &= \frac{\partial\widetilde{\mathcal{H}}(p_1,\ldots,p_N,\widetilde{p}_{N+1},q_1,\ldots,q_N,\widetilde{q}_{N+1})}{\partial p_j}, \qquad j = 1,2,\ldots,N,\end{aligned} \tag{11}$$

where

$$\widetilde{\mathcal{H}}(p_1,\ldots,p_N,\widetilde{p}_{N+1},q_1,\ldots,q_N,\widetilde{q}_{N+1}) = \frac{\mathcal{H}(p_1,\ldots p_{N+1},q_1,\ldots q_{N+1})}{v(p_1,\ldots,p_N,q_1,\ldots,q_N)} \tag{12}$$

is a dual Hamiltonian of $\mathcal{H}(p_1,\ldots p_{N+1},q_1,\ldots q_{N+1})$.

If the Hamiltonian $\widetilde{\mathcal{H}}(p_1,\ldots p_{N+1},q_1,\ldots q_{N+1})$ has singularities, the Hamiltonian system (6) has singularities. The behaviours of (6) in neighbourhoods of singularities are not simulated without loss of information by using numerical integrators. This is why the function $v(p_1,\ldots,p_N,q_1,\ldots,q_N)$ should be selected on the phase space $\mathcal{M}$ so that the Hamiltonian $\mathcal{H}(p_1,\ldots p_{N+1},q_1,\ldots q_{N+1})$ has no singularities.

The extended canonical transformation (8) on $\mathcal{M}_{\mathcal{E}}$ transforms the given Hamiltonian system (6) to (11). If (6) is a Stäckel system, then so is (11). Consequently, (8) is a canonical transformation between two different Stäckel systems. We here restrict ourselves to this case. Such a transformation is performed by using a function $v = v(q_1, \ldots, q_N)$ which does not depend on $p_1, \ldots, p_N$.

Proposition 2 (Tsiganov [29])**.** *If the two Stäckel matrices* $\mathbf{S}$ *and* $\widetilde{\mathbf{S}}$ *are distinguished by the first row only, namely,*

$$s_{k,j} = \widetilde{s}_{k,j}, \qquad k \neq 1, \tag{13}$$

the corresponding Hamiltonians I_1 *and* $\widetilde{I}_1$ *with a common set of potentials* $U_j(q_j)$ *are mutually related by the following extended canonical transformation on the extended phase space* $\mathcal{M}_{\mathcal{E}}$*:*

$$\begin{aligned} &I_1 = H(p_1, \ldots, p_N, q_1, \ldots, q_N) \\ &\mapsto \widetilde{I}_1 = \widetilde{H}(p_1, \ldots, p_N, q_1, \ldots, q_N) = \frac{I_1}{v(q_1, \ldots, q_N)}, \\ &\mathrm{d}t \mapsto \mathrm{d}\widetilde{t} = v(q_1, \ldots, q_N)\, \mathrm{d}t, \end{aligned} \tag{14}$$

where $v(q_1, \ldots, q_N)$ *is given by a ratio of determinants of the Stäckel matrices*

$$v(q_1, \ldots, q_N) = \frac{\det \widetilde{\mathbf{S}}(q_1, \ldots, q_N)}{\det \mathbf{S}(q_1, \ldots, q_N)}. \tag{15}$$

The extended Hamiltonian $\mathcal{H}(p_1, \ldots, p_N, p_{N+1}, q_1, \ldots, q_N, q_{N+1})$ satisfying condition (7) is transformed to $\widetilde{\mathcal{H}}(p_1, \ldots, p_N, \widetilde{p}_{N+1}, q_1, \ldots, q_N, \widetilde{q}_{N+1})$, a dual Hamiltonian, satisfying

$$\widetilde{\mathcal{H}}(p_1, \ldots, p_N, \widetilde{p}_{N+1}, q_1, \ldots, q_N, \widetilde{q}_{N+1}) \equiv 0. \tag{16}$$

From (5), (9) and (14) we obtain

$$\widetilde{\mathcal{H}}(p_1, \ldots, p_N, \widetilde{p}_{N+1}, q_1, \ldots, q_N, \widetilde{q}_{N+1}) = \widetilde{H}(p_1, \ldots, p_N, q_1, \ldots, q_N) - \widetilde{E} \equiv 0. \tag{17}$$

Let $\widetilde{H}(p_1, \ldots, p_N, q_1, \ldots, q_N)$ be a Hamiltonian of a given Stäckel system. Theorem 1 with (3) implies that there exists a dual Stäckel system having a Hamiltonian

$$I_1 = H(p_1, \ldots, p_N, q_1, \ldots, q_N) = \sum_{k=1}^{N} c_{k,1} \left(p_k^2 + U_k(q_k) \right), \qquad c_{k,1} = \frac{\partial \log \det \mathbf{S}}{\partial s_{1,k}}. \tag{18}$$

In the subsequent subsections we consider three Hamiltonian systems as important examples of the Stäckel system [29, 30]. The canonical variables in Hamiltonians are separated explicitly by certain extended canonical transformation of type (14).

2.3. Kepler motion in three-dimensional space as Stäckel system

We briefly review that the three-dimensional Kepler motion is an example of Stäckel systems. Through the canonical transformation on $\mathcal{M}$ called the KS regularization transformation [1, 17, 28]

$$\begin{aligned} &x = q_1^2 - q_2^2 - q_3^2 + q_4^2, \qquad y = 2(q_1 q_2 - q_3 q_4), \qquad z = 2(q_1 q_3 + q_2 q_4), \\ &p_x = \frac{1}{2} \frac{p_1 q_1 - p_2 q_2 - p_3 q_3 + p_4 q_4}{q_1^2 + q_2^2 + q_3^2 + q_4^2}, \qquad p_y = \frac{1}{2} \frac{p_1 q_2 + p_2 q_1 - p_3 q_4 - p_4 q_3}{q_1^2 + q_2^2 + q_3^2 + q_4^2}, \\ &p_z = \frac{1}{2} \frac{p_1 q_3 + p_2 q_4 + p_3 q_1 + p_4 q_2}{q_1^2 + q_2^2 + q_3^2 + q_4^2}, \qquad p_1 q_4 - p_2 q_3 + p_3 q_2 - p_4 q_1 = 0, \end{aligned} \tag{19}$$

the zero-valued extended Hamiltonian of the three-dimensional Kepler motion

$$\mathcal{H}_{\text{kepl-1}}(p_x, p_y, p_z, -E_{\text{kepl}}, x, y, z, \widetilde{t}) = \frac{1}{2}\left(p_x^2 + p_y^2 + p_z^2\right) - \frac{K^2}{\sqrt{x^2+y^2+z^2}} - E_{\text{kepl}} \equiv 0 \quad (20)$$

leads to the extended Hamiltonian

$$\begin{aligned}\mathcal{H}_{\text{kepl-2}}&(p_1, p_2, p_3, p_4, -E_{\text{kepl}}, q_1, q_2, q_3, q_4, \widetilde{t})\\ &= \frac{1}{8}\frac{p_1^2 + p_2^2 + p_3^2 + p_4^2 + U(q_1) + U(q_2) + U(q_3) + U(q_4)}{q_1^2+q_2^2+q_3^2+q_4^2} \equiv 0,\end{aligned} \quad (21)$$

where

$$U(q_j) = -8E_{\text{kepl}}q_j^2 - 2K^2, \qquad j = 1, \ldots, 4, \quad (22)$$

where $\tilde{t}$ is the time variable of the three-dimensional Kepler motion, K^2 is a given positive constant and E_{kepl} is the constant satisfying (20). We have some choices of (q_1, q_2, q_3, q_4) corresponding to (x, y, z), since one of the variables q_1, q_2, q_3, q_4 is arbitrary. An example of choice is shown in [1], p 57.

We see that the system with Hamiltonian (21) is the very Stäckel system. Four constants of motion are given by

$$\begin{pmatrix}\widetilde{I}_1\\ \widetilde{I}_2\\ \widetilde{I}_3\\ \widetilde{I}_4\end{pmatrix} = \left(\widetilde{\mathbf{S}}_{\text{kepl}}^{-1}\right)^{\top}\begin{pmatrix}p_1^2 + U(q_1)\\ p_2^2 + U(q_2)\\ p_3^2 + U(q_3)\\ p_4^2 + U(q_4)\end{pmatrix}, \quad (23)$$
$$\widetilde{I}_1 = \mathcal{H}_{\text{kepl-2}}(p_1, p_2, p_3, p_4, -E_{\text{kepl}}, q_1, q_2, q_3, q_4, \widetilde{t}),$$

where the corresponding Stäckel matrix $\widetilde{\mathbf{S}}_{\text{kepl}}$ is

$$\widetilde{\mathbf{S}}_{\text{kepl}} = \begin{pmatrix}8q_1^2 & 8q_2^2 & 8q_3^2 & 8q_4^2\\ 1 & -1 & 0 & 0\\ 0 & 1 & -1 & 0\\ 0 & 0 & 1 & -1\end{pmatrix}. \quad (24)$$

On the other hand, the four-dimensional harmonic oscillator is a Stäckel system, whose Hamiltonian is the sum of one-dimensional Hamiltonian systems. The four-dimensional oscillator has the Hamiltonian

$$\begin{aligned}&\mathcal{H}_{\text{osc}}(p_1, p_2, p_3, p_4, -E_{\text{osc}}, q_1, q_2, q_3, q_4, t) = \tfrac{1}{4}\left(p_1^2 + p_2^2 + p_3^2 + p_4^2\right) - 2K^2 - E_{\text{osc}},\\ &E_{\text{osc}} = 2E_{\text{kepl}}\left(q_1^2 + q_2^2 + q_3^2 + q_4^2\right),\end{aligned} \quad (25)$$

where K^2 is a given positive constant in (20). The time variable of the four-dimensional oscillator is t. $\mathcal{H}_{\text{osc}}(p_1, p_2, p_3, p_4, -E_{\text{osc}}, q_1, q_2, q_3, q_4, t)$ satisfies the zero Hamiltonian condition because of

$$\begin{aligned}\mathcal{H}_{\text{osc}}&(p_1, p_2, p_3, p_4, -E_{\text{osc}}, q_1, q_2, q_3, q_4, t)\\ &= 2\left(q_1^2 + q_2^2 + q_3^2 + q_4^2\right)\mathcal{H}_{\text{kepl-2}}(p_1, p_2, p_3, p_4, -E_{\text{kepl}}, q_1, q_2, q_3, q_4, \tilde{t}) \equiv 0.\end{aligned} \quad (26)$$

The Hamiltonian system has four constants of motion I_k described by

$$\begin{pmatrix} I_1 \\ I_2 \\ I_3 \\ I_4 \end{pmatrix} = \left(\mathbf{S}_{\mathrm{kepl}}^{-1}\right)^{\top} \begin{pmatrix} p_1^2 + U(q_1) \\ p_2^2 + U(q_2) \\ p_3^2 + U(q_3) \\ p_4^2 + U(q_4) \end{pmatrix}, \tag{27}$$
$$I_1 = \mathcal{H}_{\mathrm{osc}}(p_1, p_2, p_3, p_4, -E_{\mathrm{osc}}, q_1, q_2, q_3, q_4, t),$$

where the Stäckel matrix $\mathbf{S}_{\mathrm{kepl}}$ is given by

$$\mathbf{S}_{\mathrm{kepl}} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 1 & -1 \end{pmatrix}. \tag{28}$$

The two different dynamical systems (21) and (25) have a common set of potentials $U(q_i), i = 1, \ldots, 4$, and correspond to the Stäckel matrices $\mathbf{S}_{\mathrm{kepl}}, \widetilde{\mathbf{S}}_{\mathrm{kepl}}$, respectively, which are different by the first row. Proposition 2 implies that $\mathcal{H}_{\mathrm{osc}}(p_1, p_2, p_3, p_4, -E_{\mathrm{osc}}, q_1, q_2, q_3, q_4, t)$ and $\mathcal{H}_{\mathrm{kepl\text{-}2}}(p_1, p_2, p_3, p_4, -E_{\mathrm{kepl}}, q_1, q_2, q_3, q_4, \widetilde{t})$ are related by an extended canonical transformation on $\mathcal{M}_{\mathcal{E}}$. The result is as follows:

$$\begin{aligned} &I_1 = \mathcal{H}_{\mathrm{osc}}(p_1, p_2, p_3, p_4, -E_{\mathrm{osc}}, q_1, q_2, q_3, q_4, t) \\ &\mapsto \widetilde{I}_1 = \mathcal{H}_{\mathrm{kepl\text{-}2}}(p_1, p_2, p_3, p_4, -E_{\mathrm{kepl}}, q_1, q_2, q_3, q_4, \widetilde{t}) = \frac{I_1}{v_{\mathrm{kepl}}(q_1, q_2, q_3, q_4)} \\ &\mathrm{d}t \mapsto \mathrm{d}\widetilde{t} = v_{\mathrm{kepl}}(q_1, q_2, q_3, q_4)\,\mathrm{d}t, \end{aligned} \tag{29}$$

where

$$v_{\mathrm{kepl}}(q_1, q_2, q_3, q_4) = \frac{\det \widetilde{\mathbf{S}}_{\mathrm{kepl}}(q_1, \ldots, q_N)}{\det \mathbf{S}_{\mathrm{kepl}}(q_1, \ldots, q_N)} = 2\left(q_1^2 + q_2^2 + q_3^2 + q_4^2\right). \tag{30}$$

We see that the zero-valued Hamiltonian (21) is equivalent to (26) through (29). Thus, the three-dimensional Kepler motion and the four-dimensional harmonic oscillator are mutually dual Stäckel systems. The transformation from the real time $\widetilde{t}$ to the fictitious time t is sometimes called the Kepler change of the time. Under the KS canonical transformation (19) and the second canonical transformation (29), the Hamiltonian $\mathcal{H}_{\mathrm{kepl\text{-}1}}$ is regularized to $\mathcal{H}_{\mathrm{osc}}$ on the extended phase space $\mathcal{M}_{\mathcal{E}}$. Simultaneously, the Kepler motion reduces to a sequence of one-dimensional problems.

The Kepler motion with the zero-valued Hamiltonian (21) has three constants of motion as follows:

(a) the Hamiltonian $\mathcal{H}_{\mathrm{kepl\text{-}2}}(p_1, p_2, p_3, p_4, -E_{\mathrm{kepl}}, q_1, q_2, q_3, q_4, \widetilde{t})$;
(b) the angular momentum

$$\mathbf{h}_{\mathrm{kepl}}(p_1, p_2, p_3, p_4, q_1, q_2, q_3, q_4) = \frac{1}{2}\begin{pmatrix} 2l_{4,1}(p_4, p_1, q_4, q_1) \\ l_{1,3}(p_1, p_3, q_1, q_3) - l_{2,4}(p_2, p_4, q_2, q_4) \\ l_{1,2}(p_1, p_2, q_1, q_2) + l_{3,4}(p_3, p_4, q_3, q_4) \end{pmatrix}^{\top}, \tag{31}$$

where

$$l_{i,j}(p_i, p_j, q_i, q_j) = p_i q_j - p_j q_i, \qquad i, j = 1, \ldots, 4; \tag{32}$$

(c) the Runge–Lenz vector

$$\mathbf{e}_{\text{kepl}}(p_1, p_2, p_3, p_4, q_1, q_2, q_3, q_4) = \frac{1}{4}\begin{pmatrix} 32E_{\text{kepl}}\left(q_1^2 - q_2^2 - q_3^2 - q_4^2\right) - 4\left(p_1^2 - p_2^2 - p_3^2 + p_4^2\right) \\ 8E_{\text{kepl}}(q_1q_3 + q_2q_4) - (p_1p_3 + p_2p_4) \\ 8E_{\text{kepl}}(q_1q_2 - q_3q_4) - (p_1p_2 - p_3p_4) \end{pmatrix}^{\top}. \tag{33}$$

With the help of three independent constants of motion of the Hamiltonian (21) and the angular momentum (31), the Kepler motion is shown to be completely integrable. The Runge–Lenz vector (33) is an additional constant of motion which makes the Kepler motion *super-integrable* (cf [15]). Consequently, any bounded orbits are closed and periodic.

The Hamiltonian (21) is expressed as a function of $\tilde{I}_1$ in (29). Moreover, it is easy to check the conservation of angular momentum (31). By using Stäckel matrix, it is shown that (33) are the function of the constants of motion $\tilde{I}_1, \tilde{I}_2, \tilde{I}_3, \tilde{I}_4$ and the angular momentum of the harmonic oscillator $l_{1,2}, l_{1,3}, l_{1,4}, l_{2,4}, l_{3,4}$. It is clear that the angular momentum (31) is a vector-valued function of the quantities $l_{1,2}, l_{1,3}, l_{1,4}, l_{2,4}, l_{3,4}$. The x, y and z components of the Runge–Lenz vector, $(e_{\text{kepl}})_x$, $(e_{\text{kepl}})_y$ and $(e_{\text{kepl}})_z$, respectively, are given as follows:

$$\begin{aligned}
(e_{\text{kepl}})_x &= -2\tilde{I}_2 + 2\tilde{I}_4, \\
(e_{\text{kepl}})_y &= -\tfrac{1}{4}\,\text{sign}(p_1p_3 - 8\tilde{I}_1q_1q_3)\sqrt{(\tilde{I}_2 + 8K^2)(-\tilde{I}_3 + \tilde{I}_4 + 8K^2) + 8\tilde{I}_1l_{1,3}^2} \\
&\quad - \tfrac{1}{4}\,\text{sign}(p_2p_4 - 8\tilde{I}_1q_2q_4)\sqrt{(-\tilde{I}_4 + 8K^2)(-\tilde{I}_2 + \tilde{I}_3 + 8K^2) + 8\tilde{I}_1l_{2,4}^2}, \\
(e_{\text{kepl}})_z &= -\tfrac{1}{4}\,\text{sign}(p_1p_2 - 8\tilde{I}_1q_1q_2)\sqrt{(\tilde{I}_2 + 8K^2)(-\tilde{I}_2 + \tilde{I}_3 + 8K^2) + 8\tilde{I}_1l_{1,2}^2} \\
&\quad + \tfrac{1}{4}\,\text{sign}(p_3p_4 - 8\tilde{I}_1q_3q_4)\sqrt{(-\tilde{I}_4 + 8K^2)(-\tilde{I}_3 + \tilde{I}_4 + 8K^2) + 8\tilde{I}_1l_{3,4}^2}.
\end{aligned} \tag{34}$$

The conservations of $\tilde{I}_1, \tilde{I}_2, \tilde{I}_3, \tilde{I}_4, l_{1,2}, l_{1,3}, l_{1,4}, l_{2,4}, l_{3,4}$ give rise to those of the Hamiltonian (21), the angular momentum (31) and the Runge–Lenz vector (33).

2.4. *Holt system as Stäckel system*

The Holt system is a class of completely integrable two-dimensional Hamiltonian systems found by Holt [12]. Let us consider the Holt system on $\mathcal{M}_{\mathcal{E}}$ having Hamiltonian (cf [25])

$$\mathcal{H}_{\text{hlt-1}}(p_x, p_y, -E_{\text{hlt}}, x, y, \tilde{t}) = p_x^2 + p_y^2 + 4\alpha^2x^{4/3} + \tfrac{9}{4}\alpha^2x^{-2/3}y^2 + 2\beta x^{-2/3} - 2E_{\text{hlt}}, \tag{35}$$

where α, β and E_{hlt} are arbitrary the constants. We choose the constant E_{hlt} as

$$\mathcal{H}_{\text{hlt-1}}(p_x, p_y, -E_{\text{hlt}}, x, y, \tilde{t}) \equiv 0. \tag{36}$$

Here, the time variable of the Holt system is $\tilde{t}$. The extended Hamiltonian (35) is transformed into that of a Stäckel system

$$\mathcal{H}_{\text{hlt-2}}(p_1, p_2, -E_{\text{hlt}}, q_1, q_2, \tilde{t}) = \frac{p_1^2 + p_2^2 + U(q_1) + U(q_2)}{q_1 + q_2}, \tag{37}$$

where

$$U(q_j) = 4\alpha^2q_j^3 - 2E_{\text{hlt}}q_j + 2\beta, \qquad j = 1, 2, \tag{38}$$

after the canonical transformation

$$\begin{aligned}
q_1 &= x^{2/3} - \frac{1}{2\sqrt{3}\alpha}p_y, & q_2 &= x^{2/3} + \frac{1}{2\sqrt{3}\alpha}p_y, \\
p_1 &= -p_xx^{1/3} + \frac{3}{2}\alpha y, & p_2 &= -p_xx^{1/3} - \frac{3}{2}\alpha y.
\end{aligned} \tag{39}$$

The dynamical system with the Hamiltonian (37) is a Stäckel system and has two constants of motion $\widetilde{I}_k$ given by

$$\begin{aligned}
&\begin{pmatrix}\widetilde{I}_1\\ \widetilde{I}_2\end{pmatrix} = \left(\widetilde{\mathbf{S}}_{\mathrm{hlt}}^{-1}\right)^{\top}\begin{pmatrix}p_1^2+U(q_1)\\ p_2^2+U(q_2)\end{pmatrix},\\
&\widetilde{I}_1 = \mathcal{H}_{\text{hlt-2}}(p_1, p_2, -E_{\mathrm{hlt}}, q_1, q_2, \widetilde{t}),\\
&\widetilde{I}_2 = \frac{q_2}{q_1+q_2}\left(p_1^2+U(q_1)\right) - \frac{q_1}{q_1+q_2}\left(p_2^2+U(q_2)\right).
\end{aligned} \tag{40}$$

The Stäckel matrix is

$$\widetilde{\mathbf{S}}_{\mathrm{hlt}} = \begin{pmatrix} q_1 & q_2\\ 1 & -1\end{pmatrix}. \tag{41}$$

The zero Hamiltonian condition (36) gives

$$\mathcal{H}_{\text{hlt-2}}(p_1, p_2, -E_{\mathrm{hlt}}, q_1, q_2, \widetilde{t}) \equiv 0. \tag{42}$$

Let us consider another Stäckel system with the Hamiltonian

$$\begin{aligned}
&\mathcal{H}_{\text{a-osc}}(p_1, p_2, -E_s, q_1, q_2, t) = \frac{1}{2}\left(p_1^2+p_2^2+U(q_1)+U(q_2)\right),\\
&E_{\text{a-osc}} = \frac{q_1+q_2}{2}E_{\mathrm{hlt}},
\end{aligned} \tag{43}$$

where the potentials $U(q_j)$ are the same as in (38). The Hamiltonian (43) describes a two-dimensional aharmonic oscillator. Let us choose the arbitrary parameter β as

$$\mathcal{H}_{\text{a-osc}}(p_1, p_2, -E_{\text{a-osc}}, q_1, q_2, t) \equiv 0. \tag{44}$$

This system has the time variable t and two constants of motion I_k defined by

$$\begin{aligned}
&\begin{pmatrix}I_1\\ I_2\end{pmatrix} = \left(\mathbf{S}_{\mathrm{hlt}}^{-1}\right)^{\top}\begin{pmatrix}p_1^2+U(q_1)\\ p_2^2+U(q_2)\end{pmatrix},\\
&I_1 = \mathcal{H}_{\text{a-osc}}(p_1, p_2, -E_{\text{a-osc}}, q_1, q_2, t),\\
&I_2 = \frac{1}{2}\left(p_1^2+U(q_1)\right) - \frac{1}{2}\left(p_2^2+U(q_2)\right)
\end{aligned} \tag{45}$$

with the Stäckel matrix

$$\mathbf{S}_{\mathrm{hlt}} = \begin{pmatrix} 1 & 1\\ 1 & -1\end{pmatrix}. \tag{46}$$

The Holt system (37) and the Stäckel system with the Hamiltonian (43) have a common set of potentials $U(q_1)$, $U(q_2)$ and correspond to the Stäckel matrices which are different by the first row. The following relationship can be found by using proposition 2:

$$\begin{aligned}
&I_1 = \mathcal{H}_{\text{a-osc}}(p_1, p_2, -E_s, q_1, q_2, t)\\
&\quad\mapsto \widetilde{I}_1 = \mathcal{H}_{\text{hlt-2}}(p_1, p_2, -E_{\mathrm{hlt}}, q_1, q_2, \widetilde{t}) = \frac{I_1}{v_{\mathrm{hlt}}(q_1, q_2)},\\
&\mathrm{d}t \mapsto \mathrm{d}\widetilde{t} = v_{\mathrm{hlt}}(q_1, q_2)\,\mathrm{d}t,\\
&v_{\mathrm{hlt}}(q_1, q_2) = \frac{q_1+q_2}{2}.
\end{aligned} \tag{47}$$

We see that condition (44) is equivalent to (36) through (42).

2.5. Integrable Henon–Heiles system as Stäckel system

The Henon–Heiles-type system is originally known as a chaotic Hamiltonian system in celestial mechanics [9]. By a simple change of the Hamiltonian we obtain a completely integrable Henon–Heiles-type system. One of such cases (cf [25]) has the extended Hamiltonian

$$\mathcal{H}_{\text{hh-1}}(p_x, p_y, -E_{\text{hh}}, x, y, t) = p_x^2 + p_y^2 + x^2 + y^2 + \tfrac{2}{3}x^3 + 2xy^2 - E_{\text{hh}} \tag{48}$$

on $\mathcal{M}_{\mathcal{E}}$. Let us set the arbitrary constant E_{hh} as

$$\mathcal{H}_{\text{hh-1}}(p_x, p_y, -E_{\text{hh}}, x, y, t) \equiv 0. \tag{49}$$

If the coefficient of x^3 is changed to $-2/3$, (48) becomes the extended Hamiltonian of the original non-integrable Henon–Heiles system. Since the Hamiltonian $\mathcal{H}_{\text{hh-1}}$ is already regular, we write the time variable as t. A separation of variables is performed by using the linear canonical transformation on $\mathcal{M}$:

$$q_1 = \tfrac{1}{2}(x + y), \qquad q_2 = \tfrac{1}{2}(x - y), \qquad p_1 = p_x + p_y, \qquad p_2 = p_x - p_y. \tag{50}$$

The extended Hamiltonian (48) leads to

$$\mathcal{H}_{\text{hh-2}}(p_1, p_2, -E_{\text{hh}}, q_1, q_2, t) = \tfrac{1}{2}\left(p_1^2 + p_2^2 + U(q_1) + U(q_2)\right), \tag{51}$$

where the potential functions are

$$U(q_j) = \tfrac{16}{3}q_j^3 + 4q_j^2 - E_{\text{hh}}, \qquad j = 1, 2. \tag{52}$$

Hamiltonian $\mathcal{H}_{\text{hh-2}}$ means a sequence of one-dimensional Hamiltonian systems. Condition (49) implies

$$\mathcal{H}_{\text{hh-2}}(p_1, p_2, -E_{\text{hh}}, q_1, q_2, t) \equiv 0. \tag{53}$$

The dynamical system with the extended Hamiltonian (51) is a Stäckel system and has two constants of motion I_k given by

$$\begin{aligned} \begin{pmatrix} I_1 \\ I_2 \end{pmatrix} &= \left(\mathbf{S}_{\text{hh}}^{-1}\right)^{\top} \begin{pmatrix} p_1^2 + U(q_1) \\ p_2^2 + U(q_2) \end{pmatrix}, \\ I_1 &= \mathcal{H}_{\text{hh-2}}(p_1, p_2, -E_{\text{hh}}, q_1, q_2, t), \\ I_2 &= \frac{1}{2}\left(p_1^2 - p_2^2 + U(q_1) - U(q_2)\right) \end{aligned} \tag{54}$$

with the Stäckel matrix

$$\mathbf{S}_{\text{hh}} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{55}$$

3. Main theorem and new numerical integrator

As is shown in sections 2.1 and 2.2, a Hamiltonian $\widetilde{H}(p_1, \ldots, p_N, q_1, \ldots, q_N)$ of Stäckel system comes from a Hamiltonian

$$H(p_1, \ldots, p_N, q_1, \ldots, q_N) = \sum_{k=1}^{N} c_{k,1}\left(p_k^2 + U_k(q_k)\right), \qquad c_{k,1} = g_k(q_1, \ldots, q_N)$$

through an extended canonical transformation (14). From (4) the Stäckel system with $H(p_1, \ldots, p_N, q_1, \ldots, q_N)$ has the following N zero-valued constants denoted by

$$\mathcal{H}_j(p_j, q_j) = p_j^2 + F_j(q_j), \qquad j = 1, \ldots, N, \tag{56}$$

where $F_j(q_j) = U_j(q_j) - \sum_{k=1}^{N} s_{k,j}(q_j)I_k$, $j = 1, \ldots, N$. By using (5), the extended Hamiltonian $\mathcal{H}(p_1, \ldots, p_N, -I_1, q_1, \ldots, q_N, t)$ corresponding to $H(p_1, \ldots, p_N, q_1, \ldots, q_N)$ is expressed as

$$\mathcal{H}(p_1, \ldots, p_N, -I_1, q_1, \ldots, q_N, t) = \sum_{j=1}^{N} g_j(q_1, \ldots, q_N)\mathcal{H}_j(p_j, q_j). \tag{57}$$

From (6) the Hamiltonian system with the Hamiltonian $H(p_1, \ldots, p_N, q_1, \ldots, q_N)$ leads to

$$\begin{aligned} \frac{\mathrm{d}p_j}{\mathrm{d}t} &= -g_j(q_1, \ldots, q_N)\frac{\partial \mathcal{H}_j(p_j, q_j)}{\partial q_j}, \\ \frac{\mathrm{d}q_j}{\mathrm{d}t} &= g_j(q_1, \ldots, q_N)\frac{\partial \mathcal{H}_j(p_j, q_j)}{\partial p_j}, \qquad j = 1, \ldots, N. \end{aligned} \tag{58}$$

It is clear that the Hamiltonian system (58) conserves the values of $\mathcal{H}_1(p_1, q_1), \ldots, \mathcal{H}_N(p_N, q_N)$. The conservation of $I_1, \ldots, I_N$ is induced by that of $\mathcal{H}_1(p_1, q_1), \ldots, \mathcal{H}_N(p_N, q_N)$. If we apply an energy-preserving method to the Hamiltonian system (58), $\mathcal{H}_1(p_1, q_1), \ldots, \mathcal{H}_N(p_N, q_N)$ are conserved, consequently, all constants of motion $I_1, \ldots, I_N$ are also kept constant under a discrete-time evolution of the energy-preserving scheme.

From proposition 2, the Stäckel system with the Stäckel matrix $\widetilde{\mathbf{S}}$ distinguished from $\mathbf{S}$ by the first row only satisfies the following relation:

$$\widetilde{\mathbf{S}} \begin{pmatrix} \widetilde{I}_1 \\ \vdots \\ \widetilde{I}_N \end{pmatrix} = \begin{pmatrix} p_1^2 + U_1(q_1) \\ \vdots \\ p_N^2 + U_N(q_N) \end{pmatrix}, \tag{59}$$

where $\widetilde{I}_1, \ldots, \widetilde{I}_N$ are the constants of motion. By (4) and (59),

$$\mathbf{S} \begin{pmatrix} I_1 \\ \vdots \\ I_N \end{pmatrix} = \widetilde{\mathbf{S}} \begin{pmatrix} \widetilde{I}_1 \\ \vdots \\ \widetilde{I}_N \end{pmatrix} \tag{60}$$

is derived. From (56) and (60), the N zero-valued constants $\mathcal{H}_1, \ldots, \mathcal{H}_N$ are rewritten as

$$\mathcal{H}_j(p_j, q_j) = p_j^2 + \tilde{F}_j(q_j), \qquad j = 1, \ldots, N, \tag{61}$$

where $\widetilde{F}_j(q_j) = U_j(q_j) - \sum_{k=1}^{N} \widetilde{s}_{k,j}(q_j)\widetilde{I}_k$, $j = 1, \ldots, N$. As the Hamiltonian system (58) keeps the values of $\mathcal{H}_1, \ldots, \mathcal{H}_N$ zeros, those of $\widetilde{I}_1, \ldots, \widetilde{I}_N$ are conserved.

Now we are in a position to state the main theorem.

Theorem 2. *Let $\widetilde{\mathcal{H}}(p_1, \ldots, p_N, -\widetilde{I}_1, q_1, \ldots, q_N, \widetilde{t})$ and $\mathcal{H}(p_1, \ldots, p_N, -I_1, q_1, \ldots, q_N, t)$ be an extended Hamiltonian of a given Stäckel system and its dual Hamiltonian related by the extended canonical transformation (14), respectively. Assume that $\mathcal{H}(p_1, \ldots, p_N, -I_1, q_1, \ldots, q_N, t)$ is expressed as a sum of Hamiltonians of one degree of freedom such that*

$$\mathcal{H}(p_1, \ldots, p_N, -I_1, q_1, \ldots, q_N, t) = \sum_{k=1}^{N} c_{k,1}\mathcal{H}_k(p_k, q_k), \qquad \mathcal{H}_k(p_k, q_k) = p_k^2 + F_k(q_k), \tag{62}$$

where each $F_k(q_k)$ is a regular function of q_k and each $c_{k,1} = g_k(q_1, \ldots, q_N)$ is a constant. Then, an energy-preserving scheme for the Hamiltonian system (58) *induces a numerical integrator for the Hamiltonian system with the extended Hamiltonian* $\widetilde{\mathcal{H}}(p_1, \ldots, p_N, -\widetilde{I}_1, q_1, \ldots, q_N, \widetilde{t})$ *which conserves N constants of motion* $\widetilde{I}_1, \ldots, \widetilde{I}_N$.

The Kepler motion (21), the Holt system (37) and the Henon–Heiles system (51) belong to a special but important class, where $U_k(q_k) = U(q_k)$ and $c_{k,1}$ are some nonzero constants for $k = 1, 2, \ldots, N$.

We next explain how to present a new numerical integrator for Stäckel system. The new numerical integrator keeps exactly the same number of constants of motion as the degree of freedom which a Stäckel system has. These constants of motion fix a single orbit of a Stäckel system on a phase space.

In order to simulate a perturbed Kepler system, the adaptive Verlet method [19] was introduced in which the Hamiltonian of the system is split into the Kepler part and the perturbation. This method does not accurately simulate the perturbed Kepler motion because an adopted numerical integrator does not compute even the behaviour of the Kepler part accurately. An accurate numerical integrator for completely integrable system is necessary so that the behaviour of a perturbed Hamiltonian system is investigated accurately. Hence, even an completely integrable system needs an accurate numerical integrator.

The algorithm for numerical integration of Stäckel system is described as follows:

(0) Introduce a Hamiltonian on an extended phase space $\mathcal{M}_{\mathcal{E}}$. Fix the value of an arbitrary constant in the extended Hamiltonian which corresponds to energy level by the zero Hamiltonian condition.

(i) Find a canonical transformation on $\mathcal{M}$ such that the extended Hamiltonian is transformed into that of a Stäckel system.

(ii) If the Hamiltonian of the Stäckel system in (i) is not regular at some point of phase space, this system can be transformed to another Stäckel system whose Hamiltonian is regular in the whole phase space by the inverse of an extended canonical transformation on $\mathcal{M}_{\mathcal{E}}$. Simultaneously, the time variable $\widetilde{t}$ is changed to a fictitious time t. Find such an extended canonical transformation. Then the canonical variables of the Hamiltonian are separated. If the Hamiltonian of the Stäckel system in (i) is regular in the whole phase space and separated without using any canonical transformation, then go to (iii).

(iii) Discretize the Hamiltonian system with a regular Hamiltonian, which is the sum of one-dimensional Hamiltonian systems, by a variant of the energy-preserving methods.

(iv) Derive a discrete-time dynamical system from that given in (iii) by using a discrete counterpart of the extended canonical transformations of (ii).

(v) A new numerical integrator is obtained from the discrete-time dynamical system in (iv) after the inverse of the canonical transformation in (i).

The resulting numerical integrator remarkably conserves the same number of constants of motion as the degree of freedom of the original dynamical system. Our new numerical integrator has its base not only on the regularization theory but also on separation of variables for Stäckel system. This fundamental property is not perceived well in the previous works [22, 23]. Note that the Levi-Civita transformation used in [22] and the KS transformation in [23] are examples of the canonical transformation in (i). The transformation in (ii) is the inverse of the extended canonical transformations (14) given by proposition 2. The time variable is changed in general after the extended canonical transformation in (iv). Therefore, a discrete-time system having variable time step-size naturally appears. In the next section, we apply the new numerical integration algorithm to the Kepler motion, the Holt system and the integrable Henon–Heiles system concretely.

In this paper, we adopt Greenspan's energy-preserving method [4, 5] with a variable step-size

$$\begin{aligned} \frac{P_k^{(j+1)} - P_k^{(j)}}{s^{(j+1)} - s^{(j)}} &= -c_{k,1} \frac{F_k\big(Q_k^{(j+1)}\big) - F_k\big(Q_k^{(j)}\big)}{Q_k^{(j+1)} - Q_k^{(j)}}, \\ \frac{Q_k^{(j+1)} - Q_k^{(j)}}{s^{(j+1)} - s^{(j)}} &= c_{k,1}\big(P_k^{(j+1)} + P_k^{(j)}\big) \end{aligned} \tag{63}$$

for (58). Here, $s^{(j)}$ is a discrete-time variable which is given as an arbitrarily increasing sequence and corresponds to the continuous-time variable t. The variables $P_k^{(j)}, Q_k^{(j)}$ correspond to p_k, q_k and are the values of P_k, Q_k at the time $s^{(j)}$ such that

$$P_k^{(0)} = p_k(0), \qquad Q_k^{(0)} = q_k(0). \tag{64}$$

As the system (63) keeps the values of $\mathcal{H}_1\big(P_1^{(j)}, Q_1^{(j)}\big), \dots, \mathcal{H}_N\big(P_N^{(j)}, Q_N^{(j)}\big)$ zeros, it has N constants of motion $\tilde{I}_1\big(P_1^{(j)}, Q_1^{(j)}\big), \dots, \tilde{I}_N\big(P_N^{(j)}, Q_N^{(j)}\big)$. Since the integrable Henon–Heiles system can be transformed to a regular and Stäckel system directly by a single canonical transformation, steps (ii) and (iv) can be omitted to present a numerical integrator for the Henon–Heiles system. The zero Hamiltonian conditions are useful not only to find the duality of two Stäckel systems but also to determine orbits of the resulting discrete-time integrable systems by using given initial data, where each orbit is distinguished by the value of the constant in (0).

Remark 1. If we adopt the symplectic scheme (cf [8, 26]) in step (iii), the resulting integrator does not conserve all the constants of motion anymore. In order to draw an orbit, for example, an orbit near a critical point such as a separatrix, we need an exactly conserving integrator.

4. Discrete-time systems derived from Stäckel systems

In this section, we derive new discretizations of three completely integrable systems discussed in section 2. The Roman numbers (0), (i) , . . . , (v) mean the steps of the new numerical integration algorithm.

4.1. Discrete Kepler motion

4.1.1. Numerical integrator for three-dimensional Kepler motion.

(0) The constant E_{kepl} in the extended Hamiltonian $\mathcal{H}_{\text{kepl-1}}$ is fixed by the zero Hamiltonian condition (7).

(i) The Hamiltonian (20) leads to the Hamiltonian $\mathcal{H}_{\text{kepl-2}}$ in (21) after the KS canonical transformation (19). The Hamiltonian system corresponding to the Hamiltonian (21) is

$$\begin{aligned} \frac{\mathrm{d}q_k}{\mathrm{d}\tilde{t}} &= \frac{1}{4}\frac{p_k}{q_1^2 + q_2^2 + q_3^2 + q_4^2}, \\ \frac{\mathrm{d}p_k}{\mathrm{d}\tilde{t}} &= \frac{1}{4}\frac{\big(p_1^2 + p_2^2 + p_3^2 + p_4^2\big) - 8K^2}{\big(q_1^2 + q_2^2 + q_3^2 + q_4^2\big)^2} q_k, \qquad k = 1, \dots, 4, \end{aligned} \tag{65}$$

where $\tilde{t}$ is the time variable. This is a Stäckel system.

(ii) The Stäckel system given in (i) has the Stäckel matrix (24). The Hamiltonian of this system is not regular at the origin $q_1 = q_2 = q_3 = q_4 = 0$. It follows from proposition 2 that this Stäckel system leads to the four-dimensional harmonic oscillator with the time variable t. The resulting Hamiltonian $\mathcal{H}_{\rm osc}$ in (25) is regular in the whole phase space. The Hamiltonian system of the four-dimensional oscillator is

$$\frac{{\rm d}q_k}{{\rm d}t} = \frac{1}{4}p_k, \qquad \frac{{\rm d}p_k}{{\rm d}t} = 2E_{\rm kepl}q_k, \qquad k = 1,\ldots,4, \tag{66}$$

where we use $\mathcal{H}_{\text{kepl-2}} \equiv 0$ for $E_{\rm kepl}$. This system is corresponding to the Stäckel matrix (28). The four-dimensional oscillator and the Hamiltonian system (65) are directly related by the extended canonical transformation (29).

(iii) The Hamiltonian system of the four-dimensional oscillator (25) is discretized by the energy-preserving method with a variable step-size (cf [4, 5, 10]) as follows:

$$\begin{aligned}&\frac{Q_k^{(j+1)} - Q_k^{(j)}}{s^{(j+1)} - s^{(j)}} = \frac{P_k^{(j)} + P_k^{(j+1)}}{8}, \qquad \frac{P_k^{(j+1)} - P_k^{(j)}}{s^{(j+1)} - s^{(j)}} = E_{\rm kepl}\big(Q_k^{(j)} + Q_k^{(j+1)}\big),\\ &P_k^{(0)} = p_k(0), \qquad Q_k^{(0)} = q_k(0), \qquad k = 1,\ldots,4.\end{aligned} \tag{67}$$

On the orbit of the discrete-time four-dimensional harmonic oscillator (67), the Hamiltonian $\mathcal{H}_{\rm osc}$ in (25) takes a constant value for any $s^{(j)}$, namely,

$$\begin{aligned}&\mathcal{H}_{\rm osc}\big(P_1^{(j+1)}, P_2^{(j+1)}, P_3^{(j+1)}, P_4^{(j+1)}, -E_{\rm osc}, Q_1^{(j+1)}, Q_2^{(j+1)}, Q_3^{(j+1)}, Q_4^{(j+1)}, s^{(j+1)}\big)\\ &\qquad = \mathcal{H}_{\rm osc}(P_1^{(j)}, P_2^{(j)}, P_3^{(j)}, P_4^{(j)}, -E_{\rm osc}, Q_1^{(j)}, Q_2^{(j)}, Q_3^{(j)}, Q_4^{(j)}, s^{(j)}),\\ &j = 0, 1, \ldots.\end{aligned} \tag{68}$$

It follows from (26) that $\mathcal{H}_{\rm osc} = 0$ at $t = 0$. Thus, we see

$$\mathcal{H}_{\rm osc}\big(P_1^{(j)}, P_2^{(j)}, P_3^{(j)}, P_4^{(j)}, -E_{\rm osc}, Q_1^{(j)}, Q_2^{(j)}, Q_3^{(j)}, Q_4^{(j)}, t^{(j)}\big) \equiv 0, \qquad j = 0, 1, \ldots. \tag{69}$$

From (64) and (25) we can get the expression of the constant $E_{\rm kepl}$ as follows:

$$E_{\rm kepl} = \frac{1}{8}\frac{\big(P_1^{(0)}\big)^2 + \big(P_2^{(0)}\big)^2 + \big(P_3^{(0)}\big)^2 + \big(P_4^{(0)}\big)^2 - 8K^2}{\big(Q_1^{(0)}\big)^2 + \big(Q_2^{(0)}\big)^2 + \big(Q_3^{(0)}\big)^2 + \big(Q_4^{(0)}\big)^2}. \tag{70}$$

(iv) We introduce a new discrete-time variable $\widetilde{s}^{(j)}$, $j = 0, 1, \ldots,$ defined by

$$\widetilde{s}^{(j+1)} - \widetilde{s}^{(j)} = 2\big(\big(Q_1^{(j)}\big)^2 + \big(Q_2^{(j)}\big)^2 + \big(Q_3^{(j)}\big)^2 + \big(Q_4^{(j)}\big)^2\big)(s^{(j+1)} - s^{(j)}), \tag{71}$$

where (71) is a discrete analogue to the Kepler change of the time (29). By using (71), we see that the discrete-time four-dimensional oscillator (67) is transformed into

$$\begin{aligned}&\frac{Q_k^{(j+1)} - Q_k^{(j)}}{\widetilde{s}^{(j+1)} - \widetilde{s}^{(j)}} = \frac{1}{16}\frac{P_k^{(j)} + P_k^{(j+1)}}{\big(Q_1^{(j)}\big)^2 + \big(Q_2^{(j)}\big)^2 + \big(Q_3^{(j)}\big)^2 + \big(Q_4^{(j)}\big)^2},\\ &\frac{P_k^{(j+1)} - P_k^{(j)}}{\widetilde{s}^{(j+1)} - \widetilde{s}^{(j)}} = \frac{1}{2}\frac{E_{\rm kepl}\big(Q_k^{(j)} + Q_k^{(j+1)}\big)}{\big(Q_1^{(j)}\big)^2 + \big(Q_2^{(j)}\big)^2 + \big(Q_3^{(j)}\big)^2 + \big(Q_4^{(j)}\big)^2},\\ &\qquad k = 1,\ldots,4, \qquad j = 0, 1, \ldots.\end{aligned} \tag{72}$$

Moreover, (71) gives a discrete analogue of the extended canonical transformation (29):

$$\begin{aligned}&\mathcal{H}_{\rm osc}\big(P_1^{(j)}, P_2^{(j)}, P_3^{(j)}, P_4^{(j)}, -E_{\rm osc}, Q_1^{(j)}, Q_2^{(j)}, Q_3^{(j)}, Q_4^{(j)}, s^{(j)}\big)\\ &\qquad \mapsto \mathcal{H}_{\text{kepl-2}}\big(P_1^{(j)}, P_2^{(j)}, P_3^{(j)}, P_4^{(j)}, -E_{\rm kepl}, Q_1^{(j)}, Q_2^{(j)}, Q_3^{(j)}, Q_4^{(j)}, \widetilde{s}^{(j)}\big)\\ &\qquad = \frac{\mathcal{H}_{\rm osc}\big(P_1^{(j)}, P_2^{(j)}, P_3^{(j)}, P_4^{(j)}, -E_{\rm osc}, Q_1^{(j)}, Q_2^{(j)}, Q_3^{(j)}, Q_4^{(j)}, \widetilde{s}^{(j)}\big)}{v_{\rm kepl}\big(Q_1^{(j)}, Q_2^{(j)}, Q_3^{(j)}, Q_4^{(j)}\big)},\\ &s^{(j+1)} - s^{(j)} \mapsto \widetilde{s}^{(j+1)} - \widetilde{s}^{(j)} = v_{\rm kepl}\big(Q_1^{(j)}, Q_2^{(j)}, Q_3^{(j)}, Q_4^{(j)}\big)(s^{(j+1)} - s^{(j)}),\end{aligned} \tag{73}$$

where

$$v_{\rm kepl}\big(Q_1^{(j)}, Q_2^{(j)}, Q_3^{(j)}, Q_4^{(j)}\big) = 2\big(\big(Q_1^{(j)}\big)^2 + \big(Q_2^{(j)}\big)^2 + \big(Q_3^{(j)}\big)^2 + \big(Q_4^{(j)}\big)^2\big). \tag{74}$$

Equations (72) keep the values of $\tilde{I}_1\big(P_1^{(j)}, Q_1^{(j)}\big), \ldots, \tilde{I}_4\big(P_4^{(j)}, Q_4^{(j)}\big)$ in (23). We name (72) the *shape three-dimensional discrete Kepler motion*.

(v) By using the KS canonical transformation (19), we see that the discrete Kepler motion (72) can be rewritten explicitly by using the variables in the XYZ-space:

$$P_X^{(j)}, P_Y^{(j)}, P_Z^{(j)}, X^{(j)}, Y^{(j)}, Z^{(j)}, P_X^{(j+1)}, P_Y^{(j+1)}, P_Z^{(j+1)}, X^{(j+1)}, Y^{(j+1)}, Z^{(j+1)}.$$

However, the resulting equations look too complicated to write.

Remark 2. The discrete Kepler motion (72) with (70) presents an explicit scheme with a variable step-size for a numerical integration of the three-dimensional Kepler motion.

Remark 3. Introduce a new discrete-time variable $\widetilde{s}^{(j)}$, $j = 0, 1, \ldots,$ defined by

$$\begin{aligned}\widetilde{s}^{(j+1)} - \widetilde{s}^{(j)} = \tfrac{1}{2}\big(\big(Q_1^{(j)} + Q_1^{(j+1)}\big)^2 + \big(Q_2^{(j)} + Q_2^{(j+1)}\big)^2 + \big(Q_3^{(j)} + Q_3^{(j+1)}\big)^2 \\ + \big(Q_4^{(j)} + Q_4^{(j+1)}\big)^2\big) \times \big(s^{(j+1)} - s^{(j)}\big),\end{aligned} \tag{75}$$

in (iv) instead of (71). Then, the resulting discrete-time four-dimensional oscillator has a time-reversibility. The change of the time (75) itself is the same as in Leimkuhler [19]. Though the time-reversible integrator found in [11, 19] also conserves all constants of motion, it is an implicit scheme and costs more time than an explicit integrator in general.

4.1.2. Properties of discrete Kepler motion. As was shown in (iv), $\mathcal{H}_{\text{kepl-2}}$ is constant under the time evolution of (72). Though the conservation of the Runge–Lenz vector under the time evolution of (72) is checked by a direct calculation in [23], the reason is not explained well. We here show that the conservation of the quantities $\tilde{I}_k$ and $l_{i,j}$ gives rise to the conservation of the Runge–Lenz. This fact is revealed by representing the Kepler motion in Stäckel form.

Proposition 3. *The discrete Kepler motion (72) is an explicit scheme with a variable step-size and has three constants of motion defined as follows:*

(a) A discrete analogue of the Hamiltonian

$$\begin{aligned}&\mathcal{H}_{\text{d-kepl}}\big(P_1^{(j)}, P_2^{(j)}, P_3^{(j)}, P_4^{(j)}, Q_1^{(j)}, Q_2^{(j)}, Q_3^{(j)}, Q_4^{(j)}\big) \\ &\quad = \mathcal{H}_{\text{kepl-2}}\big(P_1^{(j)}, P_2^{(j)}, P_3^{(j)}, P_4^{(j)}, -E_{\rm kepl}, Q_1^{(j)}, Q_2^{(j)}, Q_3^{(j)}, Q_4^{(j)}, \widetilde{s}^{(j)}\big).\end{aligned} \tag{76}$$

(b) A discrete analogue of the angular momentum

$$\begin{aligned}&\mathbf{h}_{\text{d-kepl}}\big(P_1^{(j)}, P_2^{(j)}, P_3^{(j)}, P_4^{(j)}, Q_1^{(j)}, Q_2^{(j)}, Q_3^{(j)}, Q_4^{(j)}\big) \\ &\quad = \mathbf{h}_{\rm kepl}\big(P_1^{(j)}, P_2^{(j)}, P_3^{(j)}, P_4^{(j)}, Q_1^{(j)}, Q_2^{(j)}, Q_3^{(j)}, Q_4^{(j)}\big),\end{aligned} \tag{77}$$

where the definition of $\mathbf{h}_{\rm kepl}$ *is in (31).*

(c) A discrete analogue of the Runge–Lenz vector

$$\begin{aligned}&\mathbf{e}_{\text{d-kepl}}\big(P_1^{(j)}, P_2^{(j)}, P_3^{(j)}, P_4^{(j)}, Q_1^{(j)}, Q_2^{(j)}, Q_3^{(j)}, Q_4^{(j)}\big) \\ &\quad = \mathbf{e}_{\rm kepl}\big(P_1^{(j)}, P_2^{(j)}, P_3^{(j)}, P_4^{(j)}, Q_1^{(j)}, Q_2^{(j)}, Q_3^{(j)}, Q_4^{(j)}\big),\end{aligned} \tag{78}$$

where the definition of $\mathbf{e}_{\rm kepl}$ *is in (33).*

Proof.

(a) It is clear that $\mathcal{H}_{\text{kepl-2}}\big(P_1^{(j)}, P_2^{(j)}, P_3^{(j)}, P_4^{(j)}, -E_{\text{kepl}}, Q_1^{(j)}, Q_2^{(j)}, Q_3^{(j)}, Q_4^{(j)}, \widetilde{s}^{(j)}\big)$ is conserved by the new numerical integrator (see (iv)). By using definition (76), we see that

$$\mathcal{H}_{\text{d-kepl}}\big(P_1^{(j)}, P_2^{(j)}, P_3^{(j)}, P_4^{(j)}, Q_1^{(j)}, Q_2^{(j)}, Q_3^{(j)}, Q_4^{(j)}\big) \equiv 0, \qquad j = 0, 1, \ldots.$$

(b) It is easy to check the conservation of $l_{i,j}, i, j = 1, \ldots, 4$ (32), by (72). Because of this conservation, it is clear that $\mathbf{h}_{\text{d-kepl}}\big(P_1^{(j)}, P_2^{(j)}, P_3^{(j)}, P_4^{(j)}, Q_1^{(j)}, Q_2^{(j)}, Q_3^{(j)}, Q_4^{(j)}\big)$ is conserved.

(c) As shown in (34), the Runge–Lenz vector (78) is the function of quantities $\tilde{I}_1\big(P_1^{(j)}, Q_1^{(j)}\big)$, $\tilde{I}_2\big(P_2^{(j)}, Q_2^{(j)}\big)$, $\tilde{I}_3\big(P_3^{(j)}, Q_3^{(j)}\big)$, $\tilde{I}_4\big(P_4^{(j)}, Q_4^{(j)}\big)$ and $l_{1,2}\big(P_1^{(j)}, P_2^{(j)}, Q_1^{(j)}, Q_2^{(j)}\big)$, $l_{1,3}\big(P_1^{(j)}, P_3^{(j)}, Q_1^{(j)}, Q_3^{(j)}\big)$, $l_{1,4}\big(P_1^{(j)}, P_4^{(j)}, Q_1^{(j)}, Q_4^{(j)}\big)$, $l_{2,4}\big(P_2^{(j)}, P_4^{(j)}, Q_2^{(j)}, Q_4^{(j)}\big)$, $l_{3,4}\big(P_3^{(j)}, P_4^{(j)}, Q_3^{(j)}, Q_4^{(j)}\big)$. Each quantity is conserved by the discrete Kepler motion (72). Consequently, the Runge–Lenz vector (78) should be conserved. □

Hence, the discrete Kepler motion (72) exactly conserves all of the constants of motion of the continuous-time three-dimensional Kepler motion, especially, the Runge–Lenz vector. As is explained in the introduction, this property is somewhat different from the known numerical integration schemes of the Kepler motion, for example, a symplectic scheme [34, 35], an explicit variable step-size scheme [11]. We have already shown that the three-dimensional discrete Kepler motion (72) is numerically stable for any step-size in [23]. Since the Kepler motion has more constants of motion than the degree of freedom, it is an example of a super-integrable system. In the Kepler case, the new integrator conserves more constants of motion than degree of freedom.

4.1.3. Numerical example for discrete Kepler motion. Figure 1 gives a numerical example for the three-dimensional discrete Kepler motion (72) with $K = 1$ and the same discrete step-size $s^{(j+1)} - s^{(j)} = \delta$. The symbol ($\times$) indicates the orbit with $\delta = 1$. The line describes the orbit with $\delta = 0.1$. The common initial value is $X^{(0)} = 0.4, Y^{(0)} = -0.1, Z^{(0)} = 0.2, P_X^{(0)} = 0.2, P_Y^{(0)} = -0.1$, and the positive constant $P_Z^{(0)}$ is determined from the given $E_{\text{kepl}}, X^{(0)}, \ldots, P_Y^{(0)}$ through

$$\mathcal{H}_{\text{kepl-1}}\big(P_X^{(0)}, P_Y^{(0)}, P_Z^{(0)}, -E_{\text{kepl}}, X^{(0)}, Y^{(0)}, Z^{(0)}, 0\big) = 0.$$

In figure 1, the orbit corresponding to $E_{\text{kepl}} = -0.2$ traces the ellipse, the orbit of the continuous-time Kepler motion, for rather big discrete step-size. See [23] for comparisons with other numerical integrators.

4.2. Discrete Holt system

4.2.1. Numerical integrator for Holt system.

(0) The constant E_{hlt} in the extended Hamiltonian $\mathcal{H}_{\text{hlt-1}}$ is fixed by the zero Hamiltonian condition (36).

(i) The Hamiltonian (35) leads to the Hamiltonian (37) after the canonical transformation (39). The Hamiltonian system corresponding to (37) is

$$\frac{\mathrm{d}q_k}{\mathrm{d}\widetilde{t}} = \frac{2p_k}{q_1 + q_2}, \qquad \frac{\mathrm{d}p_k}{\mathrm{d}\widetilde{t}} = \frac{2E_{\text{hlt}} - 12\alpha^2 q_k^2}{q_1 + q_2}, \qquad k = 1, 2, \tag{79}$$

where $\widetilde{t}$ is the time variable. This is a Stäckel system.

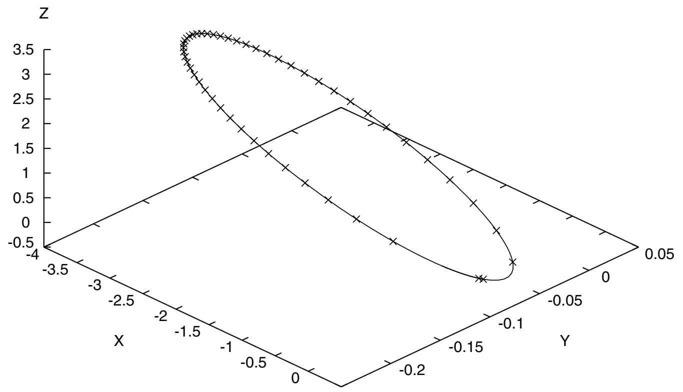

Figure 1. Three-dimensional discrete Kepler motion $\delta = 0.1, 1$.

(ii) The Stäckel system given in (i) is corresponding to the Stäckel matrix (41). The Hamiltonian (37) is not regular along the line $q_1 + q_2 = 0$. From proposition 2, the Stäckel system (79) leads to the system corresponding to the Hamiltonian $\mathcal{H}_{\text{a-osc}}(p_1, p_2, -E_s, q_1, q_2, s^{(j)})$ in (43). Here t is the time variable. The Hamiltonian $\mathcal{H}_{\text{a-osc}}$ is regular in the whole space. The resulting Hamiltonian system is an aharmonic oscillator:

$$\frac{\mathrm{d}q_k}{\mathrm{d}t} = p_k, \qquad \frac{\mathrm{d}p_k}{\mathrm{d}t} = E_{\text{hlt}} - 6\alpha^2 q_k^2, \qquad k = 1, 2. \tag{80}$$

This system has the Stäckel matrix (46). The relationship between the Holt system and the Hamiltonian system (80) is expressed with (47).

(iii) The Hamiltonian system (79) is discretized by the energy-preserving method (cf [4, 5, 10]) as follows:

$$\begin{aligned}
&\frac{Q_k^{(j+1)} - Q_k^{(j)}}{s^{(j+1)} - s^{(j)}} = \frac{P_k^{(j)} + P_k^{(j+1)}}{2},\\
&\frac{P_k^{(j+1)} - P_k^{(j)}}{s^{(j+1)} - s^{(j)}} = E_{\text{hlt}} - 2\alpha^2\left(\left(Q_k^{(j+1)}\right)^2 + \left(Q_k^{(j+1)}\right)\left(Q_k^{(j)}\right) + \left(Q_k^{(j)}\right)^2\right),\\
&s^{(0)} < \cdots < s^{(j-1)} < s^{(j)} < s^{(j+1)} < \cdots, \qquad k = 1, 2.
\end{aligned} \tag{81}$$

Here, $s^{(j)}$ is a discrete-time variable and $P_k^{(j)}$, $Q_k^{(j)}$ are the discrete variables such that $P_k^{(0)} = p_k(0)$, $Q_k^{(0)} = q_k(0)$, respectively. On the orbit of the discrete-time system (81), the Hamiltonian (43) takes a constant value for any $s^{(j)}$, namely,

$$\begin{aligned}
&\mathcal{H}_{\text{a-osc}}\left(P_1^{(j+1)}, P_2^{(j+1)}, -E_s, Q_1^{(j+1)}, Q_2^{(j+1)}, s^{(j+1)}\right)\\
&\qquad = \mathcal{H}_{\text{a-osc}}\left(P_1^{(j)}, P_2^{(j)}, -E_s, Q_1^{(j)}, Q_2^{(j)}, s^{(j)}\right), \qquad j = 0, 1, \ldots.
\end{aligned} \tag{82}$$

Condition (44) implies $\mathcal{H}_{\text{a-osc}}\left(P_1^{(j)}, P_2^{(j)}, -E_s, Q_1^{(j)}, Q_2^{(j)}, s^{(j)}\right) \equiv 0$. From (82) we can get the value of the constant E_{hlt} as follows:

$$E_{\text{hlt}} = \frac{\left(P_1^{(0)}\right)^2 + \left(P_2^{(0)}\right)^2 + 4\alpha^2\left(\left(Q_1^{(0)}\right)^3 + \left(Q_2^{(0)}\right)^3\right)}{2\left(Q_1^{(0)} + Q_2^{(0)}\right)}. \tag{83}$$

(iv) We introduce a new discrete-time variable $\widetilde{s}^{(j)}$, $j = 0, 1, \ldots$, defined by

$$\widetilde{s}^{(j+1)} - \widetilde{s}^{(j)} = \frac{Q_1^{(j)} + Q_2^{(j)}}{2}\left(s^{(j+1)} - s^{(j)}\right), \tag{84}$$

where (84) is a discrete analogue to (47). By using (47), we see that the discrete-time aharmonic oscillator (81) is transformed into

$$\frac{Q_k^{(j+1)} - Q_k^{(j)}}{\widetilde{s}^{(j+1)} - \widetilde{s}^{(j)}} = \frac{P_k^{(j+1)} + P_k^{(j)}}{Q_1^{(j)} + Q_2^{(j)}},$$
$$\frac{P_k^{(j+1)} - P_k^{(j)}}{\widetilde{s}^{(j+1)} - \widetilde{s}^{(j)}} = \frac{2E_{\mathrm{hlt}} - 4\alpha^2\left(\left(Q_k^{(j+1)}\right)^2 + Q_k^{(j+1)}Q_k^{(j)} + \left(Q_k^{(j)}\right)^2\right)}{Q_1^{(j)} + Q_2^{(j)}},$$
$$k = 1, 2. \tag{85}$$

Moreover, (84) gives the correspondence

$$\mathcal{H}_{\text{a-osc}}\left(P_1^{(j)}, P_2^{(j)}, -E_s, Q_1^{(j)}, Q_2^{(j)}, s^{(j)}\right) \mapsto \mathcal{H}_{\text{hlt-2}}\left(P_1^{(j)}, P_2^{(j)}, -E_{\mathrm{hlt}}, Q_1^{(j)}, Q_2^{(j)}, \widetilde{s}^{(j)}\right)$$
$$= \frac{\mathcal{H}_{\text{a-osc}}\left(P_1^{(j)}, P_2^{(j)}, -E_{\text{a-osc}}, Q_1^{(j)}, Q_2^{(j)}, s^{(j)}\right)}{v_{\mathrm{hlt}}\left(Q_1^{(j)}, Q_2^{(j)}\right)},$$
$$s^{(j+1)} - s^{(j)} \mapsto \widetilde{s}^{(j+1)} - \widetilde{s}^{(j)} = v_{\mathrm{hlt}}\left(Q_1^{(j)}, Q_2^{(j)}\right)\left(s^{(j+1)} - s^{(j)}\right), \tag{86}$$

where

$$v_{\mathrm{hlt}}\left(Q_1^{(j)}, Q_2^{(j)}\right) = \frac{Q_1^{(j)} + Q_2^{(j)}}{2}. \tag{87}$$

Equations (85) keep the value of $\mathcal{H}_{\text{hlt-2}}\left(P_1^{(j)}, P_2^{(j)}, -E_{\mathrm{hlt}}, Q_1^{(j)}, Q_2^{(j)}, \widetilde{s}^{(j)}\right)$ zero. We call (85) the *discrete Holt system*.

(v) Using the inverse of the canonical transformation (39), a discrete Holt system on the XY-plane is derived from (85).

Remark 4. Introducing a new discrete-time variable $\widehat{s}^{(j)}$, $j = 0, 1, \ldots,$ defined by

$$\widetilde{s}^{(j+1)} - \widetilde{s}^{(j)} = \frac{\left(Q_1^{(j)} + Q_1^{(j+1)}\right) + \left(Q_2^{(j)} + Q_2^{(j)}\right)}{4}\left(s^{(j+1)} - s^{(j)}\right), \tag{88}$$

in (iv), the derived discrete-time two-dimensional oscillator has a time-reversible variable step-size.

4.2.2. Constants of motion of discrete Holt system. The discrete Holt system (85) has two constants of motion as follows:

(a) A discrete analogue of the Hamiltonian:

$$\mathcal{H}_{\text{d-hlt}}\left(P_X^{(j)}, P_Y^{(j)}, X^{(j)}, Y^{(j)}\right) = \mathcal{H}_{\text{hlt-1}}\left(P_X^{(j)}, P_Y^{(j)}, -E_{\mathrm{hlt}}, X^{(j)}, Y^{(j)}, \widetilde{s}^{(j)}\right). \tag{89}$$

(b) A discrete analogue of the constant of motion $\widetilde{I}_2$ in (40):

$$\widetilde{I}_{2,\text{d-hlt-1}}\left(P_X^{(j)}, P_Y^{(j)}, X^{(j)}, Y^{(j)}\right) = \frac{\left(P_X^{(j)}\right)^2 P_Y^{(j)}}{2\sqrt{3}\alpha} + \frac{\left(P_Y^{(j)}\right)^3}{3\sqrt{3}\alpha} - \frac{4\alpha P_Y^{(j)}(X^{(j)})^{4/3}}{\sqrt{3}}$$
$$- 3\alpha P_X^{(j)}(X^{(j)})^{1/3}Y^{(j)} + \frac{3\sqrt{3}\alpha(X^{(j)})^{-2/3}(Y^{(j)})^2 P_Y^{(j)}}{8} + \frac{\beta(X^{(j)})^{-3/2}P_Y^{(j)}}{\sqrt{3}\alpha}. \tag{90}$$

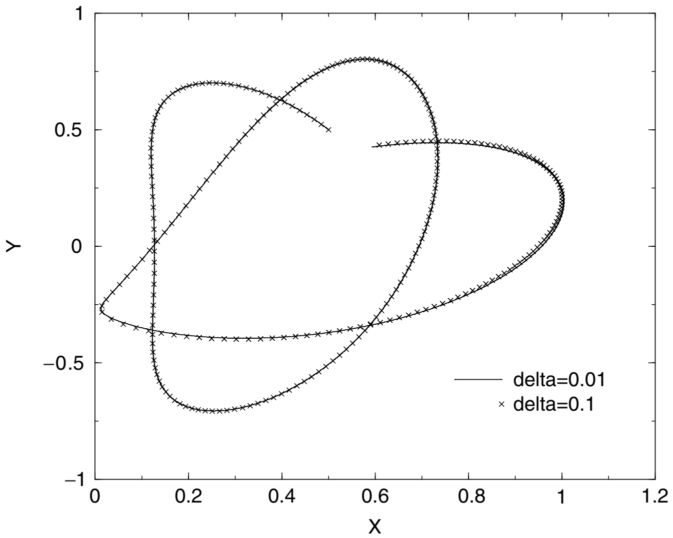

Figure 2. Discrete Holt system $\delta = 0.01, 0.1$.

We can easily prove that (81) keep $\widetilde{I}_1$ and $\widetilde{I}_2$ in (40) constant. After the inverse canonical transformation of (39), we see that $\widetilde{I}_1$ and $\widetilde{I}_2$ lead to the right-hand sides of (89) and (90), respectively. Since

$$\widetilde{I}_1 = \mathcal{H}_{\text{hlt-2}}\big(P_1^{(j)}, P_2^{(j)}, -E_{\text{hlt}}, Q_1^{(j)}, Q_2^{(j)}, \widetilde{s}^{(j)}\big)$$
$$= \mathcal{H}_{\text{hlt-1}}\big(P_X^{(j)}, P_Y^{(j)}, -E_{\text{hlt}}, X^{(j)}, Y^{(j)}, \widetilde{s}^{(j)}\big),$$
$$\widetilde{I}_2 = \widetilde{I}_{2,\text{d-hlt-1}}\big(P_X^{(j)}, P_Y^{(j)}, X^{(j)}, Y^{(j)}\big),$$

it follows that (89) and (90) are constants of motion of the discrete Holt system (85).

4.2.3. Numerical example for discrete Holt system. A numerical example for the discrete Holt system is given in figure 2. The orbits of the discrete Holt system (85) with a constant discrete step-size $s^{(j+1)} - s^{(j)} = \delta = 0.01, 0.1$ are described, where the initial value is $X^{(0)} = 0.5$, $Y^{(0)} = 0.5$, $P_X^{(0)} = 1.0$, $P_Y^{(0)} = 1.0$ and the parameters are $\alpha = 1.0$ and $\beta = 100.0$.

4.3. Discrete integrable Henon–Heiles system

4.3.1. Numerical integrator for integrable Henon–Heiles system.

(0) The constant E_{hh} in the extended Hamiltonian $\mathcal{H}_{\text{hh-1}}$ is fixed by the zero Hamiltonian condition (49).

(i) The Hamiltonian (48) leads to the Hamiltonian (51) after the canonical transformation (50). The Hamiltonian system corresponding to the Hamiltonian (51) is

$$\frac{\mathrm{d}q_k}{\mathrm{d}t} = p_k, \qquad \frac{\mathrm{d}p_k}{\mathrm{d}t} = -8q_k^2 - 4q_k, \qquad k = 1, 2, \tag{91}$$

where t is the time variable. This is a Stäckel system.

(ii) The Stäckel system given in (i) has the Stäckel matrix (55). The Hamiltonian (51) is already regular in the whole phase space and the sum of one-dimensional Hamiltonian systems.

(iii) The Hamilton system (91) is discretized by the energy-preserving method as follows:

$$\begin{aligned} &\frac{Q_k^{(j+1)}-Q_k^{(j)}}{s^{(j+1)}-s^{(j)}}=\frac{P_k^{(j)}+P_k^{(j+1)}}{2},\\ &\frac{P_k^{(j+1)}-P_k^{(j)}}{s^{(j+1)}-s^{(j)}}=-\frac{8\big(\big(Q_k^{(j+1)}\big)^2+Q_k^{(j+1)}Q_k^{(j)}+\big(Q_k^{(j)}\big)^2\big)+6\big(Q_k^{(j+1)}+Q_k^{(j)}\big)}{3},\\ &s^{(0)}<\cdots<s^{(j-1)}<s^{(j)}<s^{(j+1)}<\cdots. \end{aligned} \tag{92}$$

Here, $s^{(j)}$ is a discrete-time variable and $P_k^{(j)}$, $Q_k^{(j)}$ are the values of P_k, Q_k at the time $s^{(j)}$, where we set $P_k^{(0)}=p_k(0)$, $Q_k^{(0)}=q_k(0)$, P_k and Q_k are the counterparts of the canonical variables p_k and q_k, respectively. On the orbit of the discrete-time integrable Henon–Heiles system (92), the Hamiltonian (51) takes a constant value for any $s^{(j)}$, namely,

$$\begin{aligned} &\mathcal{H}_{\text{hh-2}}\big(P_1^{(j+1)},P_2^{(j+1)},-E_{\text{hh}},Q_1^{(j+1)},Q_2^{(j+1)},s^{(j+1)}\big)\\ &\qquad=\mathcal{H}_{\text{hh-2}}\big(P_1^{(j)},P_2^{(j)},-E_{\text{hh}},Q_1^{(j)},Q_2^{(j)},s^{(j)}\big),\qquad j=0,1,\ldots. \end{aligned} \tag{93}$$

It follows from (53) with $P_k^{(0)}=p_k(0)$, $Q_k^{(0)}=q_k(0)$ that

$$\mathcal{H}_{\text{hh-2}}\big(P_1^{(j)},P_2^{(j)},-E_{\text{hh}},Q_1^{(j)},Q_2^{(j)},s^{(j)}\big)\equiv 0. \tag{94}$$

From (93) we can get the values of the constants $E_{1,\text{hh}}$ and $E_{2,\text{hh}}$ as follows:

$$E_{k,\text{hh}}=\tfrac{1}{2}\big(P_k^{(0)}\big)^2+\tfrac{8}{3}\big(Q_k^{(0)}\big)^3+2\big(Q_k^{(0)}\big)^2,\qquad k=1,2, \tag{95}$$

where $E_{\text{hh}}=E_{1,\text{hh}}+E_{2,\text{hh}}$.

(iv) Step (iv) is omitted in this case.

(v) Through the inverse of the canonical transformation (50), the discrete-time system (92) is converted to

$$\begin{aligned} &\frac{X^{(j+1)}-X^{(j)}}{s^{(j+1)}-s^{(j)}}=P_X^{(j+1)}+P_X^{(j)},\qquad \frac{Y^{(j+1)}-Y^{(j)}}{s^{(j+1)}-s^{(j)}}=P_Y^{(j+1)}+P_Y^{(j)},\\ &\frac{P_X^{(j+1)}-P_X^{(j)}}{s^{(j+1)}-s^{(j)}}=-\frac{2}{3}(((X^{(j+1)})^2+X^{(j+1)}X^{(j)}+(X^{(j)})^2)\\ &\qquad+((Y^{(j+1)})^2+Y^{(j+1)}Y^{(j)}+(Y^{(j)})^2))-(X^{(j+1)}+X^{(j)}),\\ &\frac{P_Y^{(j+1)}-P_Y^{(j)}}{s^{(j+1)}-s^{(j)}}=-\frac{2}{3}(2X^{(j+1)}Y^{(j+1)}+2X^{(j)}Y^{(j)}\\ &\qquad+X^{(j+1)}Y^{(j)}+X^{(j)}Y^{(j+1)})-(Y^{(j+1)}+Y^{(j)}). \end{aligned} \tag{96}$$

Equations (96) keep the value of $\mathcal{H}_{\text{hh-1}}\big(P_X^{(j)},P_Y^{(j)},-E_{\text{hh}},X1^{(j)},Y^{(j)},s^{(j)}\big)$ zero. We call (92) or (96) the *shape discrete integrable Henon–Heiles system.*

4.3.2. Constants of motion of discrete integrable Henon–Heiles system. The discrete integrable Henon–Heiles system (96) has the following two constants of motion defined by

(a) a discrete analogue of the Hamiltonian:

$$\mathcal{H}_{\text{d-hh-1}}\big(P_X^{(j)},P_Y^{(j)},X^{(j)},Y^{(j)}\big)=\mathcal{H}_{\text{hh-1}}\big(P_X^{(j)},P_Y^{(j)},-E_{\text{hh}},X^{(j)},Y^{(j)},s^{(j)}\big), \tag{97}$$

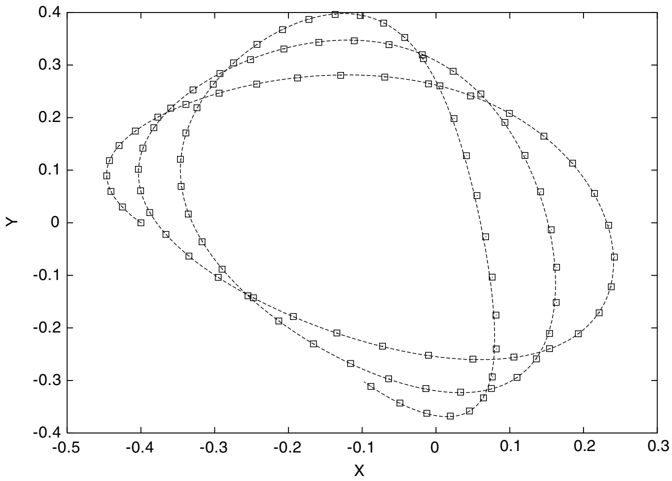

Figure 3. Discrete Henon–Heiles system $\delta = 0.01, 0.1$.

(b) a discrete analogue of the constant of motion I_2 in (54):

$$I_{2,\text{d-hh-1}}\big(P_X^{(j)}, P_Y^{(j)}, X^{(j)}, Y^{(j)}\big) = 2P_X^{(j)}P_Y^{(j)} + 4(X^{(j)})^2Y^{(j)} + \tfrac{4}{3}(Y^{(j)})^3 + 4X^{(j)}Y^{(j)} - E_{1,\text{hh}} + E_{2,\text{hh}}. \qquad (98)$$

To prove this case, we see that (92) keep I_1 and I_2 in (54) constant. After the inverse canonical transformation of (50), we see that I_1 and I_2 lead to the right-hand sides of (97) and (98), respectively. Since

$$\begin{aligned} I_1 &= \mathcal{H}_{\text{hh-2}}\big(P_1^{(j)}, P_2^{(j)}, -E_{\text{hh}}, Q_1^{(j)}, Q_2^{(j)}, s^{(j)}\big) \\ &= \mathcal{H}_{\text{hh-1}}\big(P_X^{(j)}, P_Y^{(j)}, -E_{\text{hh}}, X^{(j)}, Y^{(j)}, s^{(j)}\big), \\ I_2 &= \tfrac{1}{2}\big(\big(P_1^{(j)}\big)^2 - \big(P_2^{(j)}\big)^2\big) + \tfrac{8}{3}\big(\big(Q_1^{(j)}\big)^3 - \big(Q_2^{(j)}\big)^3\big) + 2\big(\big(Q_1^{(j)}\big)^2 - \big(Q_2^{(j)}\big)^2\big) \\ &= I_{2,\text{d-hh-1}}\big(P_X^{(j)}, P_Y^{(j)}, X^{(j)}, Y^{(j)}\big), \end{aligned}$$

(97) and (98) are shown to be constants of motion of the discrete integrable Henon–Heiles system (96).

4.3.3. Numerical example for discrete Henon–Heiles system. Finally, in this section we give a numerical example for the discrete Henon–Heiles system. Figure 3 indicates the discrete Henon–Heiles system (96) with the constant discrete step-size $s^{(j+1)} - s^{(j)} = \delta = 0.01, 0.1$, where the initial value is $X^{(0)} = -0.4$, $Y^{(0)} = 0.0$, $P_X^{(0)} = -0.15$, $P_Y^{(0)} = 0.15$. The symbol (□) indicates the orbit with $\delta = 1$. The line describes the orbit with $\delta = 0.1$.

5. Conclusion

We have proposed a new numerical integrator for a class of separable Hamiltonian systems called the Stäckel system. If the Hamiltonian of the original Stäckel system is not regular at some point, it leads to a regular and Hamiltonian of some Stäckel system through a suitable extended canonical transformation. We here adopt Greenspan's energy-preserving method as a basic numerical integration scheme. It is proved that the energy-preserving scheme induces a numerical integrator for Stäckel system conserving the same number of constants of motion as the original system (theorem 2). A successive use of

(i) a special setting of arbitrary constant in the extended Hamiltonian,
(ii) a suitable canonical transformation for the Stäckel system on an extended phase space and its inverse and
(iii) the energy-preserving method with a variable step-size

enable us to derive such an efficient numerical integrator.

We have given a new proof of the exact conservation of the constants of motion including the Runge–Lenz vector under the discrete-time evolution of the three-dimensional discrete Kepler motion (proposition 3). As a consequence, the pericentre of the elliptic orbit does not move secularly. The discrete Kepler motion has orbits which exactly trace those of the continuous-time Kepler motion, since all of the constants of motion are conserved. As a bonus, the discrete Kepler motion gives an explicit scheme with a variable step-size, which enables us a high-speed simulation of the Kepler motion with a sufficient accuracy. The discrete Holt system and the discrete integrable Henon–Heiles system are also presented. The resulting discrete-time systems have a variable step-size and keep all of the constants of motion that the continuous-time dynamical systems have. The Henon–Heiles system having the regular Hamiltonian needs a linear canonical transformation which performs a separation of variables.

The new numerical integrator has the following additional good properties: (1) coverage to the whole Stäckel system, (2) a scheme with a variable step-size and (3) a scheme with the same behaviour for large step-size. In the Kepler case, it is an explicit scheme which conserves more constants of motion than the degree of freedom. A skilful combination of a regularization technique and an energy-preserving method will be useful to discretize more wide class of dynamical systems. The authors believe that the key idea of the new numerical integrator would be valuable in many applications outside the Stäckel system, for example, to design a better solver for various n-body problems.

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